Electronic factors for isotope shifts

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The isotope shift (IS) of the frequency of a given atomic line $k$ between two isotopes $A$ and $A'$ is usually written as

$$\delta \nu_{kA,A'} = M_k \left[ \frac{(A'-A)}{AA'} \right] + F_k \delta \langle r^2 \rangle_{A,A'}$$

where the two terms represent respectively the mass shift (MS) and field shift (FS) contributions \cite{1}. $M_k$ and $F_k$ are the electronic mass and field shift factors for the considered electronic transition $k$. Using this relation, the changes in mean-square radii $\delta \langle r^2 \rangle_{A,A'}$ of the nuclear charge distribution can be determined from IS measurements provided that the electronic quantities $M_k$ and $F_k$ are known.

As far as MS are concerned, the authors of the present contribution acquired a large experience in the theoretical evaluation of the relevant parameters for highly correlated systems such as neutral atoms and negative ions (see e.g. \cite{2}). The balance between MS and FS contributions to the IS was studied for the resonance doublet lines along the lithium isoelectronic sequence \cite{3}. The “Shabaev” relativistic corrections to the recoil operator \cite{4} affecting the normal mass shift (NMS) and specific mass shift (SMS) factors contributing to $M_k$ have been implemented in the relativistic multiconfiguration Dirac-Hartree-Fock GRASP2K package \cite{5}, allowing to test the reliability of the Dirac kinetic energy operator for estimating the NMS \cite{6}.

The FS can be estimated in a perturbation approach by expressing the $F_k$ factor as proportional to the change of the electronic total probability density at the origin, calculated for a reference isotope, between the two atomic states involved in the transition, or by a variational method based on two separate electronic calculations for each level, using realistic nuclear densities for both isotopes. The difference between the two calculations reaches 5% for $^{150,142}$Nd$^{57+}$ \cite{3}. A third approach, more pragmatic, is to assume that both $M_k$ and $F_k$ factors are constants for an isotopic chain. Solving the above equation for the frequency shifts calculated by perturbation for a triplet of isotopes (or more) and using the wave functions of a given stable isotope, allows to estimate the $M_k$ and $F_k$ parameters \cite{1}.

All these computational strategies should be compared more systematically. In a joined effort, the authors will focus on some common targets, in answer to the call from the radioactive ion beam physics community who develop highly sensitive in-source laser-photoionization spectroscopy techniques, or perform laser-spectroscopic studies on short-lived radioactive nuclei to explore changes in the nuclear size, spin, and moments for isotopes far away from stability \cite{7}.

References